Department of Energy's
Innovative and Novel Computational Impact on Theory and Experiment Program

Barbara Helland

Advanced Scientific Computing Research
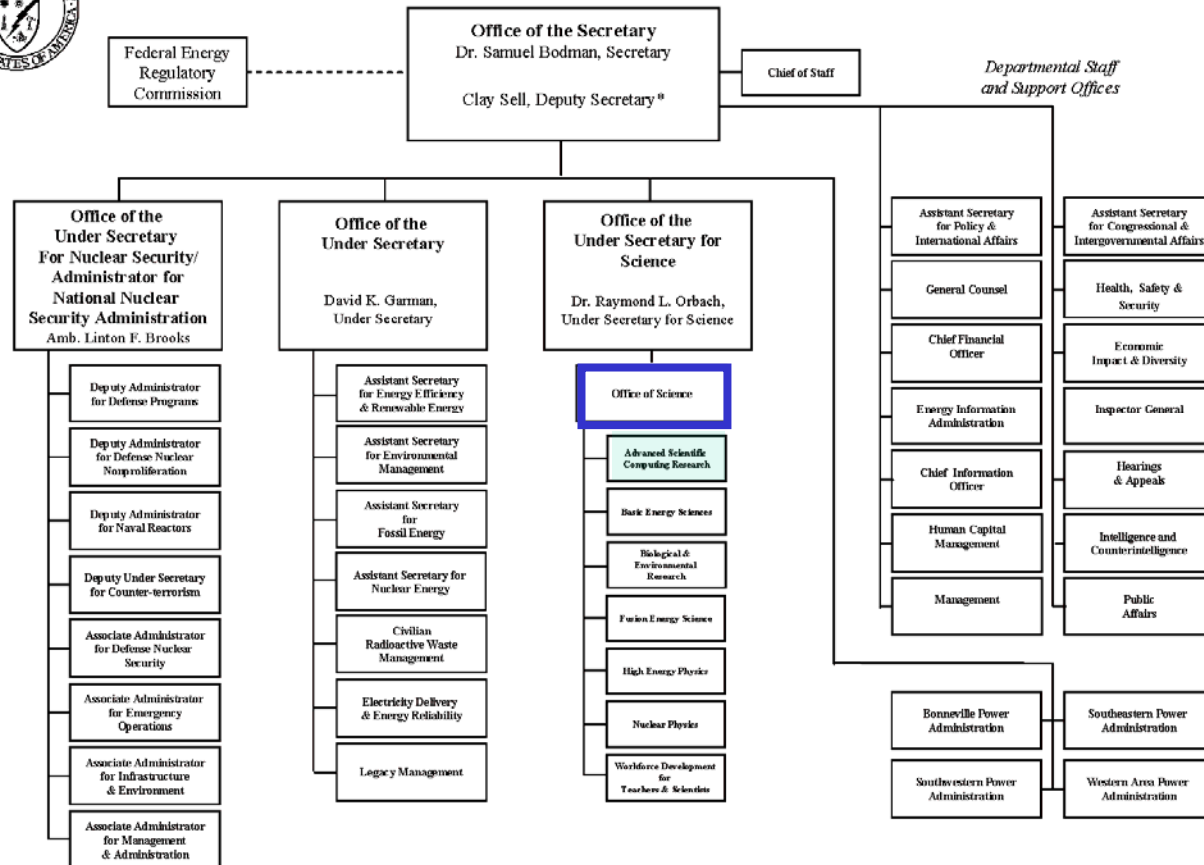
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Department of Energy Organizational Structure

Advanced Scientific Computing Research Program

DEPARTMENT OF ENERGY

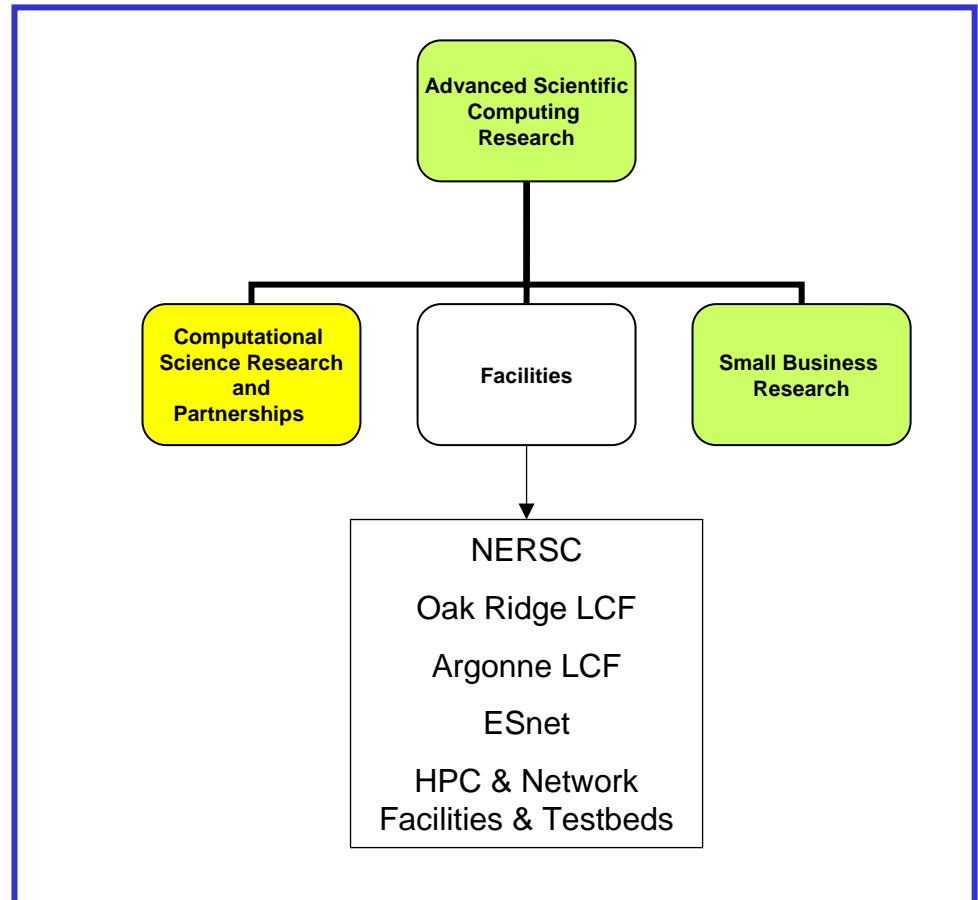* The Deputy Secretary also serves as the Chief Operating Officer

26 Oct 06

Advanced Scientific Computing Research

Advanced Scientific Computing Research Program

ASCR Mission: Steward of DOE's Computational Science, Applied Mathematics, Computer Science, High-Performance Computing and Networking Research for open science. Deploy and operate high performance computing user facilities at LBNL, ANL, and ORNL

ASCR Vision: Best in class advancing science and technological innovation through modeling and simulation

Advanced Scientific Computing Research

Computational Science Research and Partnerships — **Facilities** — **Small Business Research**

NERSC

Oak Ridge LCF

Argonne LCF

ESnet

HPC & Network Facilities & Testbeds

http://www.science.doe.gov/ascr

ASCR High Performance Computing Resources

Advanced Scientific Computing Research Program

- **High Performance Production Computing Facility (NERSC)**
  - Delivers high-end capacity computing to entire DOE SC research community
  - Large number of projects (200 – 300)
  - Medium- to very-large-scale projects that occasionally need a very high capability
  - Annual allocations

- **Leadership Computing Facilities**
  - Delivers highest computational capability to national and international researchers through peer-reviewed Innovative and Novel Computational Impact on Theory and Computation program
  - Small number of projects (10 – 20)
  - Multiple year allocations

Current Facilities

Advanced Scientific Computing Research Program

- **NERSC**
  - 10 Teraflop IBM SP 375 RS/6000 (Seaborg) with 6080 processors, 7.2 terabytes aggregate memory
  - 6.7 Teraflop IBM Power 5 (Bassi) with 888 processors, 3.5 terabytes aggregate memory
  - 3.1 Teraflop LinuxNetworx Opteron cluster (Jacquard) with 712 processors, 2.1 terabytes aggregate memory
- **LCF at Oak Ridge**
  - 119 teraflop Cray XT3/XT4 (Jaguar) with 11,708 dual core AMD Opteron processor nodes, 46 terabytes aggregate memory
  - 18.5 Teraflop Cray X1E (Phoenix) with 1,024 multi-streaming vector processors,
- **Argonne LCF**
  - 5.7 Teraflop IBM Blue Gene/L (BGL) with 2,048 PPC processors
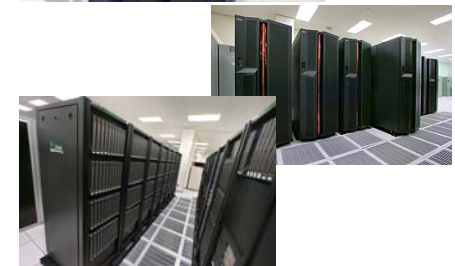
Future Facility Upgrades

Advanced Scientific Computing Research Program

- ALCF
  - 100 teraflop IBM Blue Gene/P delivered by end of 2007
  - 250-500 teraflop upgrade to IBM Blue Gene/P in late 2008
- LCF – Oak Ridge
  - Cray XT4 upgraded to 250 TF by end of 2007
  - 1 Petaflop Cray Baker system to be delivered by end of 2008
- NERSC
  - 100+ teraflop Cray XT4 in operation by October 2007

Innovative and Novel Computational Impact on Theory and Experiment-INCITE

Advanced Scientific Computing Research Program

- Initiated in 2004
- Provides Office of Science computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
- Open to national and international researchers, including industry
- No requirement of DOE Office of Science funding
- Peer and computational readiness reviewed
- 2004 Awards: 4.9 Million processor hours at NERSC awarded to three projects
- 2005 Awards: 6.5 Million processor hours at NERSC awarded to three projects

INCITE 2006

Advanced Scientific Computing Research Program

Wired Magazine, August, 2006, pg. 42
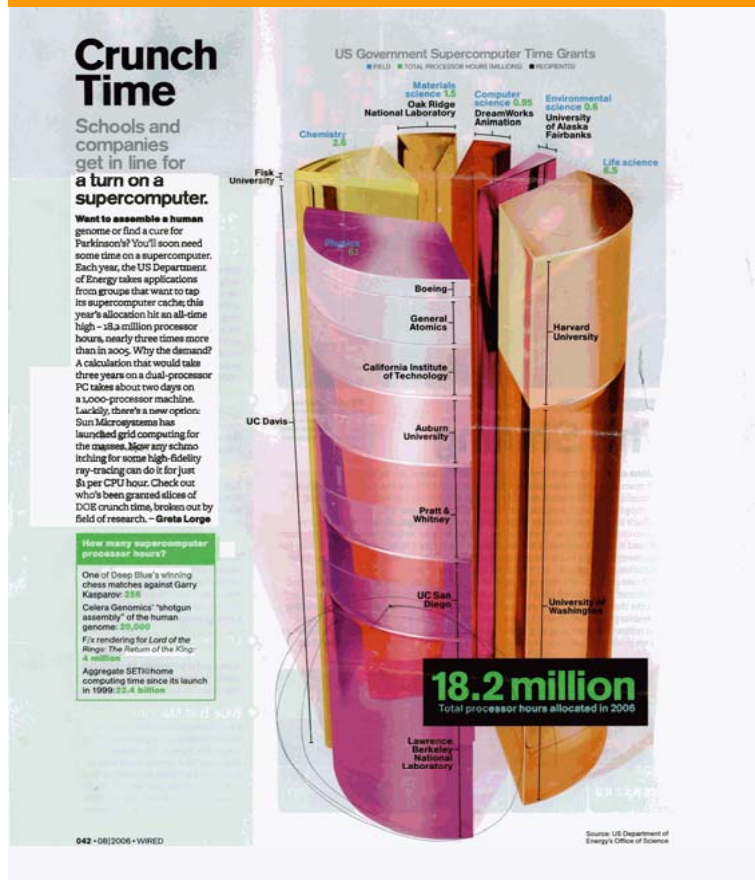
- Expanded to include SC high end computing resources at PNNL, ORNL and ANL in addition to LBNL and multiple year requests.

- Received 43 proposals requesting over 95 million processor hours.
  - 60% from Universities
  - 40% had funding from other federal research agencies

- 15 Awards for over 18.2 million processor hours

2007 INCITE Allocations by Disciplines

Advanced Scientific Computing Research Program
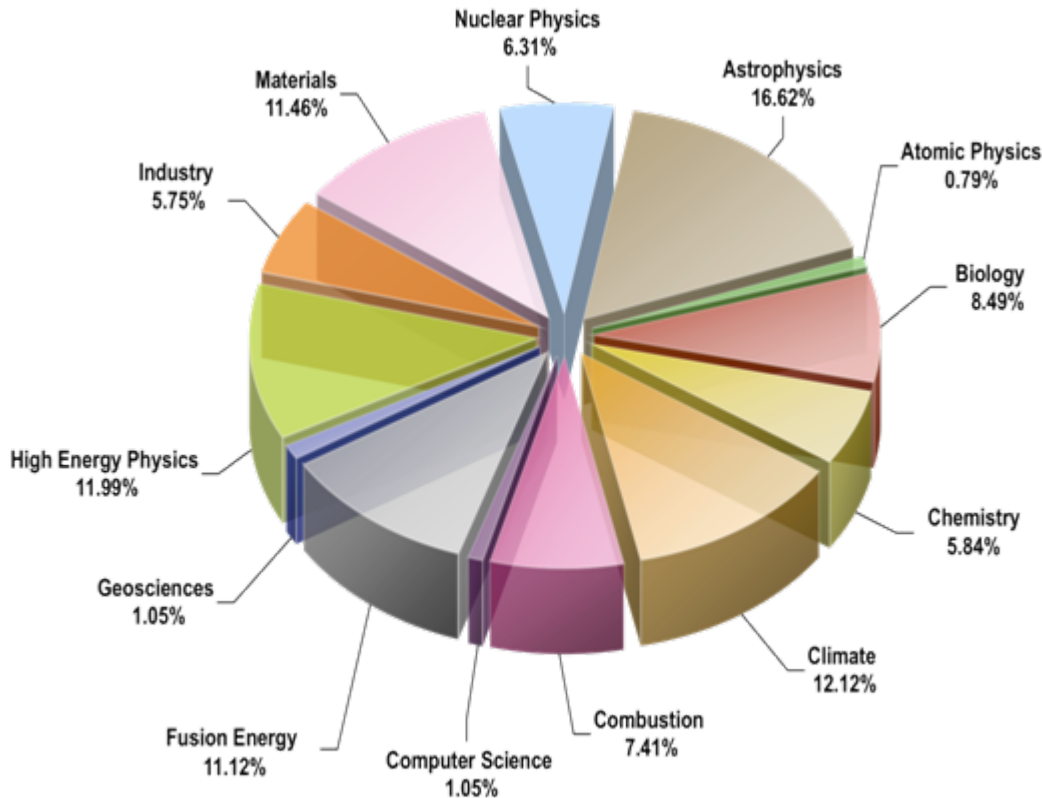
- 80% of Leadership Computing Facilities allocated through INCITE

- 88 new proposals and 20 renewal proposals received requesting over 250 Million processor hours

- 95 Million processor hours allocate to 45 projects (26 new proposals and 19 renewal)

2008 INCITE

Advanced Scientific Computing Research Program

New 2008 INCITE Call for Proposals for over 0.25 Billion processor hours

- Deadline 11:59 pm EDT August 8, 2007

- http://hpc.science.doe.gov